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MODELLING OF THE THERMOCHEMICAL PROCESSES IN THE GASIFING REACTOR USING XDEM METHOD

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Abstract. The goal of this work was to investigate the possibility of the XDEM (eXtended Discrete Element Method) program to simulate the behaviour of wood particles during the gasification process that was performed in the Institute of Fluid-Flow Machinery PASci (IMP PAN) INKA gasifier. The program is based on the Lagrangian approach for simulation of heat and mass transfer during thermal decomposition of the solid fuel particles.

1 INTRODUCTION

Typical thermochemical process of biomass in a fixed bed gasifier starts from drying, where moisture is released from fuel [1]. In the next step the volatiles are released and char is produced in the pyrolysis which occurs in the absence of oxygen. In the main gasification phase, gases are mixed with air and burned to CO_2 and H_2O. In the reduction zone charcoal combines with CO_2 and H_2O forming a combustible gas. The most important factors, which determine the composition and the quality of the syngas are the process temperature and the amount of supplied air/oxidation medium [1, 2]. Knowledge and understanding of each of these phenomena allows to get a better understanding of the whole process. This also provides to get better design and better operation parameters and, finally, better efficiency of energy conversion in the reactors.

The main goal of this work was to investigate the possibility of the XDEM program to simulate the behaviour of wood particles during the gasification process that was performed in the INKA gasifier [2].

2 XDEM METHOD

The XDEM method was developed by Peters and it aims at resolving the particulate phase with its various processes attached to the particles [3]. The main assumption of numerical modelling is that each particle undergoes a sequence of thermodynamic processes that are described by a set of one dimensional and transient conservation equations for mass, momentum and energy using Discrete Particle Method (DPM) [4, 5]. XDEM is a numerical technique that practically extends the dynamics of particles described by the classic DEM. This is graphically presented on Fig.1.

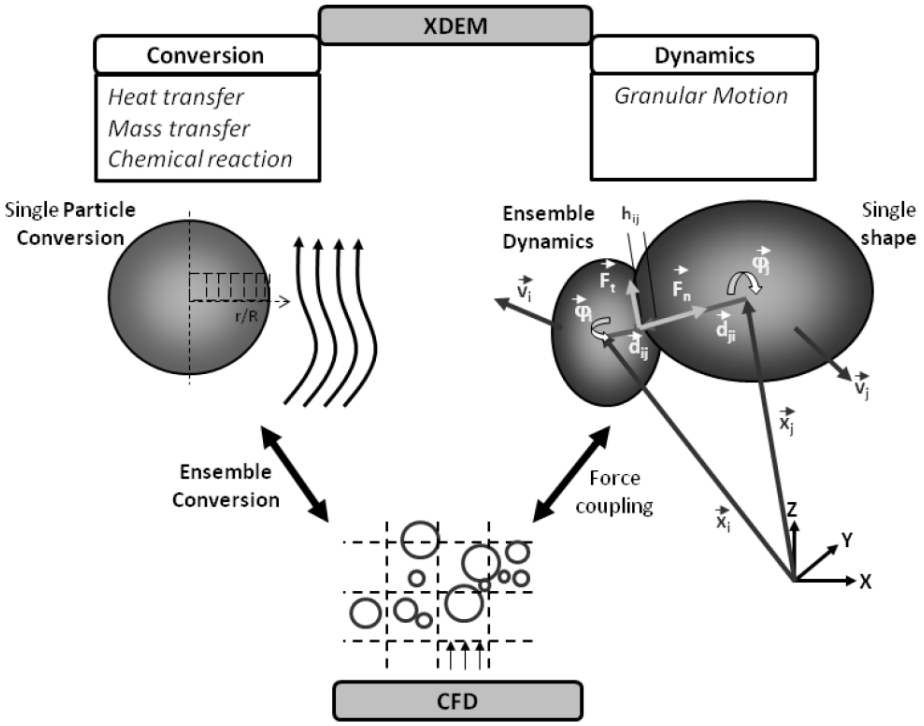

Figure 1: Scheme of the XDEM coupling with CFD [4]

While the DEM predicts position and orientation in space and time for each particle, the XDEM additionally estimates properties such as internal temperature and/or particle distribution, or mechanical impact with structures. The motion module of the DPM handles a sufficient number of geometric shapes that are believed to cover a large range of engineering applications. Relevant areas of application include furnaces for wood combustion, fluidized beds or predictions of emissions from combustion of coal or biomass. The thermodynamics module incorporates a physical-chemical approach that describes temperature and arbitrary reaction processes for each particle in an ensemble.

The coupling CFD (openFOAM solver for porous media [6]) with XDEM is realized

by the mass, momentum and heat transfer between fluid and particle part. The fluid flow is computed as a flow of gas in a porous zone, consisted of biomass particles and the gas phase filling empty spaces. The sum of all particle processes represents the overall behaviour, including heating, drying, pyrolysis and gasification.

Coupling XDEM and OpenFoam comes from the Lagrangian - Eulerian approach [4]. In Lagrangian modelling the motion and conversion of particles are computed basing on one-dimensional and transient conservation equations, which characterize energy and mass transport within each particle. It is also assumed that each particle consists of liquid, solid and gas phases, and gas is transported by diffusion and convection within the particle-pore space. All gaseous species are treated as an ideal gases and particles as an isotropic material, in which the properties may change only along the radial direction. Additionally, inside the particles there is a local thermal equilibrium between the solid and the gaseous species. Between neighbour particles heat transfer may occur through conduction and radiation. Heat and mass transfer from the fluid to the particles is computed through boundary conditions specified by the surrounding gas. Required convective heat transfer coefficients are estimated from Nusselt number semi-empirical correlation for mono-disperse and naturally arranged packed beds [7]. Appearing chemical reactions are modelled as equilibrium reactions for the available species. The motion module of DPM predicts particle positions, thus, the reactors/furnaces/boilers are naturally filled by gravity deposition.

Fluid flow is analysed based on the Eulerian approach, i.e. the fluid medium is treated as continuum. The analysed biomass/coal bed is characterized as a type of porous media in which fluid flow behaves like an external flow. Additionally, the fluid flow inside the free space is described by a three-dimensional Navier-Stokes and energy equations for incompressible flow. Moreover, Brinkmann or Forchheimer relations are used to appropriately model the drag shift from linear to non-linear behaviour. Heat and mass transfer from particle to fluid is done via source terms of the corresponding conservation equations.

3 "INKA" GASIFING REACTOR

The INKA reactor consists of one tube with three inlets at the top and one outlet at the bottom [2]. The height of the reactor is $H = 850$ mm and its diameter is $D = 206$ mm. The pipe inlets of 15 mm in diameter are located 300 mm from the top. The outlet is also a pipe with diameter of 65 mm and it is located 50 mm from the bottom. The schematic diagram of the reactor is presented on Fig.2.

In the real case, the gasifier is filled by the cuboid shape biomass particles of three different sizes, which are summarized in Tab.1. The upper level of the biomass bed is 300 mm above the air pipe inlets.

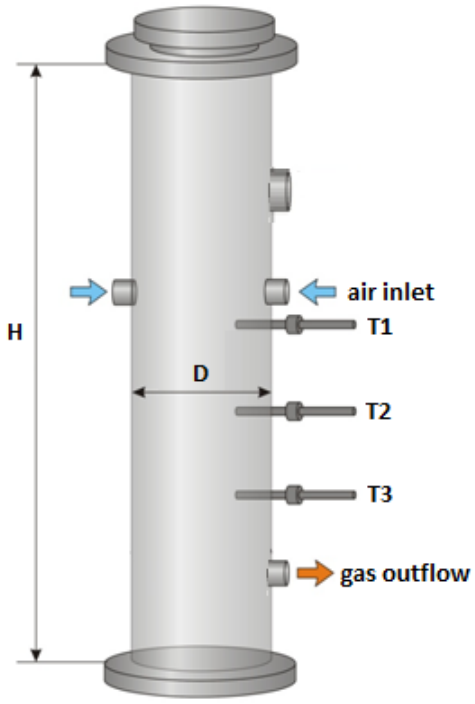

Figure 2: Scheme of the INKA gasifier INKA

Table 1: Shape parameters of the fuel wood chips

particles size	mean average size mm × mm × mm	mean volume mm^3	volume fraction %	mass fraction %
small	5 × 10 × 10	500	47	44
medium	20 × 7.5 × 6	900	29	28
large	34.5 × 18 × 15	9315	24	28

4 NUMERICAL SIMULATIONS - XDEM

Due to the fact that the real reactor is filled approximately by 35 000 particles, which is a very large number for testing case, the simplified geometry was used. It was decided to consider smaller reactor of 280 mm in height and 206 mm in diameter (Fig.3 - left picture). Because of the XDEM limitations it was assumed that the height of the CFD computational cell does not excess the value of 35 mm, which corresponds to the biggest length of the biomass block particle.

Such geometry was applied for calculation of test cases. In the first one only the flow of pure air in the small reactor was taken into account. For this purpose the *rhoPimpleFoam* solver was activated. For the second case the combustion of CH_4 in the air was considered

with only one step global reaction taken into account:

$$CH_4 + 0.5O_2 = CO_2 + 2H_2O. \quad (1)$$

For this test case the solver *reactingFoam* was used.

4.1 Filling the container

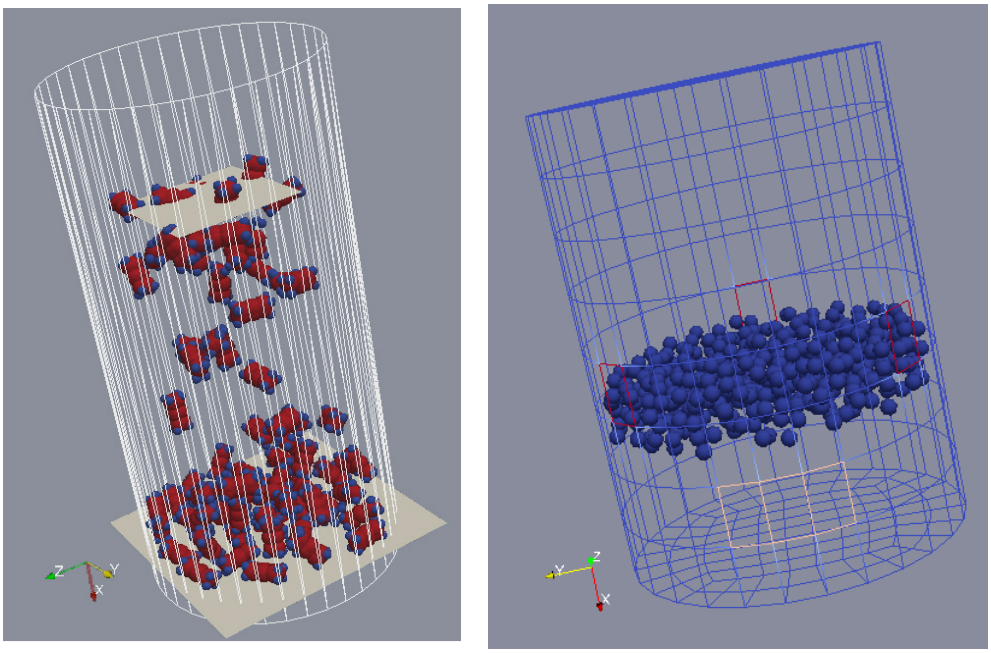

Figure 3: Filling the reactor with particles (left) and simplified geometry of the analysed geometry (right)

After CFD simulations the XDEM method (only its dynamic part) was adopted for filling the container with the particles. Two different cases were taken into account: at first step the container was filled with particles, which were of the same size (33mm x 15mm x 18mm), and with the particles of three different sizes. The calculations were stopped at certain time and the position of the particles were copied and put as an input file for coupled calculations with XDEM and OpenFOAM (Fig.3). This test case included only the drying process. After simulations the process of filling the container was repeated. Here the meshes for CFD simulations and for XDEM were ordered by choosing the same orientation direction, i.e. gravity in both cases was set according to OX direction. Now, the particles with the same and different sizes were injected into the gasifier with mass flow rate of 10 kg/s. Simulation filling time was set to 6 s and at the time of 1.8 s the injection was stopped. Following that the particles were still moved according to the process of gravitational settling on the bottom side of the reactor. The cylinder was filled approximately with 300 of biomass block particles.

After filling the container the position of the particles were copied and put as an input file to coupled calculation of XDEM and OpenFOAM. Due to the fact that the chosen shape of the particles was set as a block, the position (due to the orientation) of certain particles appeared to be unsuitable to the coupled calculation, i.e. the size of certain particles appeared to be larger than the size of the computational cell for CFD. It was decided then to change the size of mesh cells. The height of the cell was set to 45 mm, whereas the height of small reactor to 270 mm. Also the number of cells at the radial direction was reduced. To shorten the solution time the inlet and outlet boundary condition were set as a top and bottom walls of the cylinder. The simulation of drying process was repeated.

4.2 Vaporization model

Applying the reduced geometry, the coupled CFD and XDEM calculations were performed to simulate the drying process. For moisture vaporization from biomass particles the following approach was considered. It is based on balance between the energy available for evaporation and the amount of evaporated water. Thus, any heat above the evaporation temperature is available to evaporate water, which can be described as follows [8]:

$$\dot{S}_{\mathrm{H_2O}} = \begin{cases} \frac{(T-T_{evap})\rho c_p}{H_{evap}\delta t} & T \geq T_{evap} \\ 0 & T < T_{evap}, \end{cases} \tag{2}$$

where T, T_{evap}, H_{evap}, ρ, c_p, δt denote local particle temperature, evaporation temperature, evaporation enthalpy, particle density, specific heat of the particle and the time interval, respectively.

5 RESULTS

In Fig.4 and Fig.5 the XDEM/CFD numerical results are presented. In Fig.4 the propagation of the heating front in four different time steps can be observed. The fluid medium is air, which is composed from O_2 and N_2. As it can be seen the hot gas of the temperature 773 K flows into the cylinder from the top wall to the bottom wall. Gas velocity inlet v equals 2.3 m/s and operating pressure p equals 1 atm. Due to the heat transfer from hot air to cold biomass (with initial temperature of 293 K), the central temperature of each particle is increasing.

In Fig.4 the changes of the moisture content in each particle in four different time steps are presented. In this test case the initial moisture content in each particle is very small. Due to the heat propagation the particles are heated up, which leads to the water vaporization.

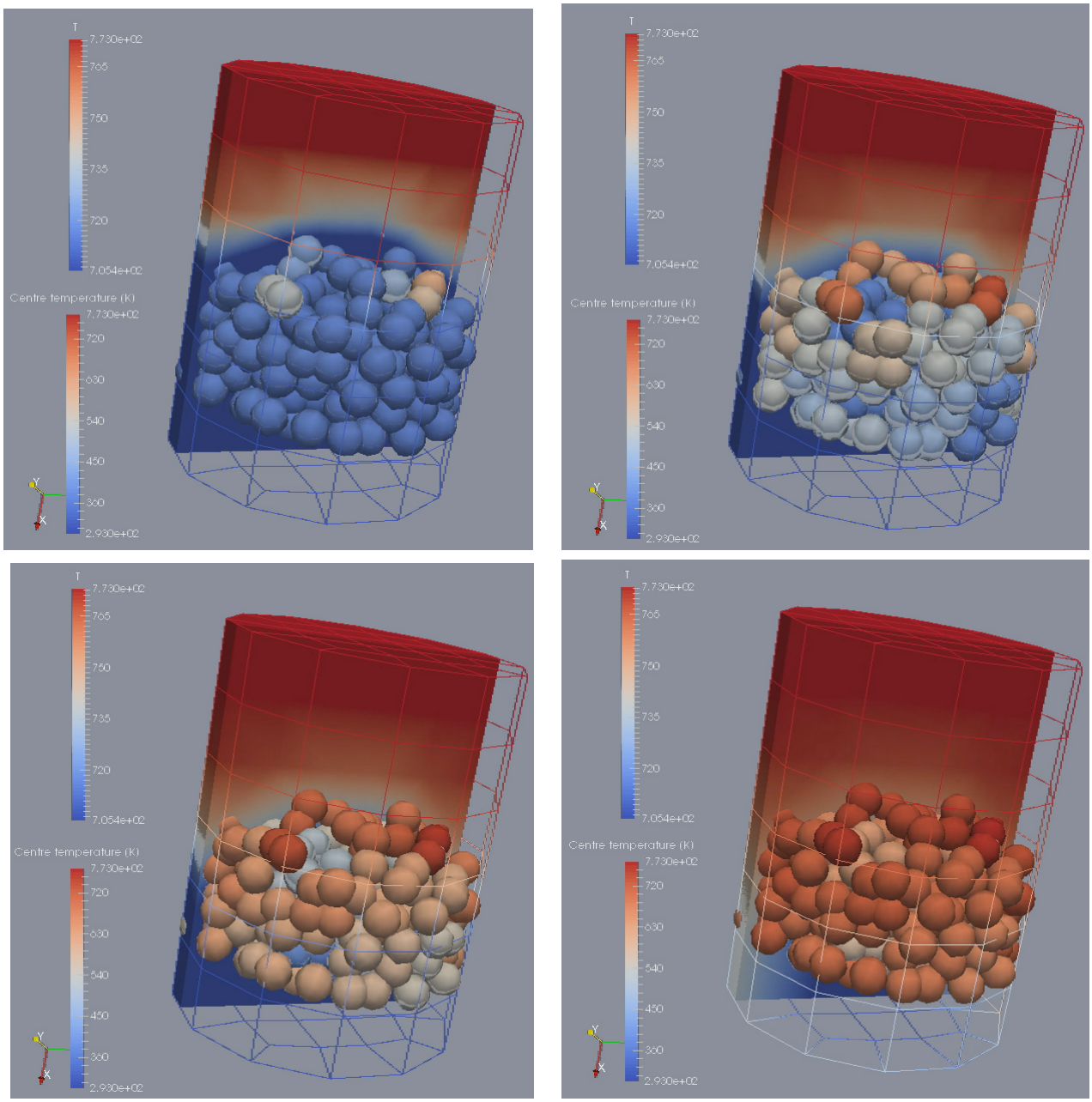

Figure 4: Temperature distribution in different time steps in the simplified analysed reactor

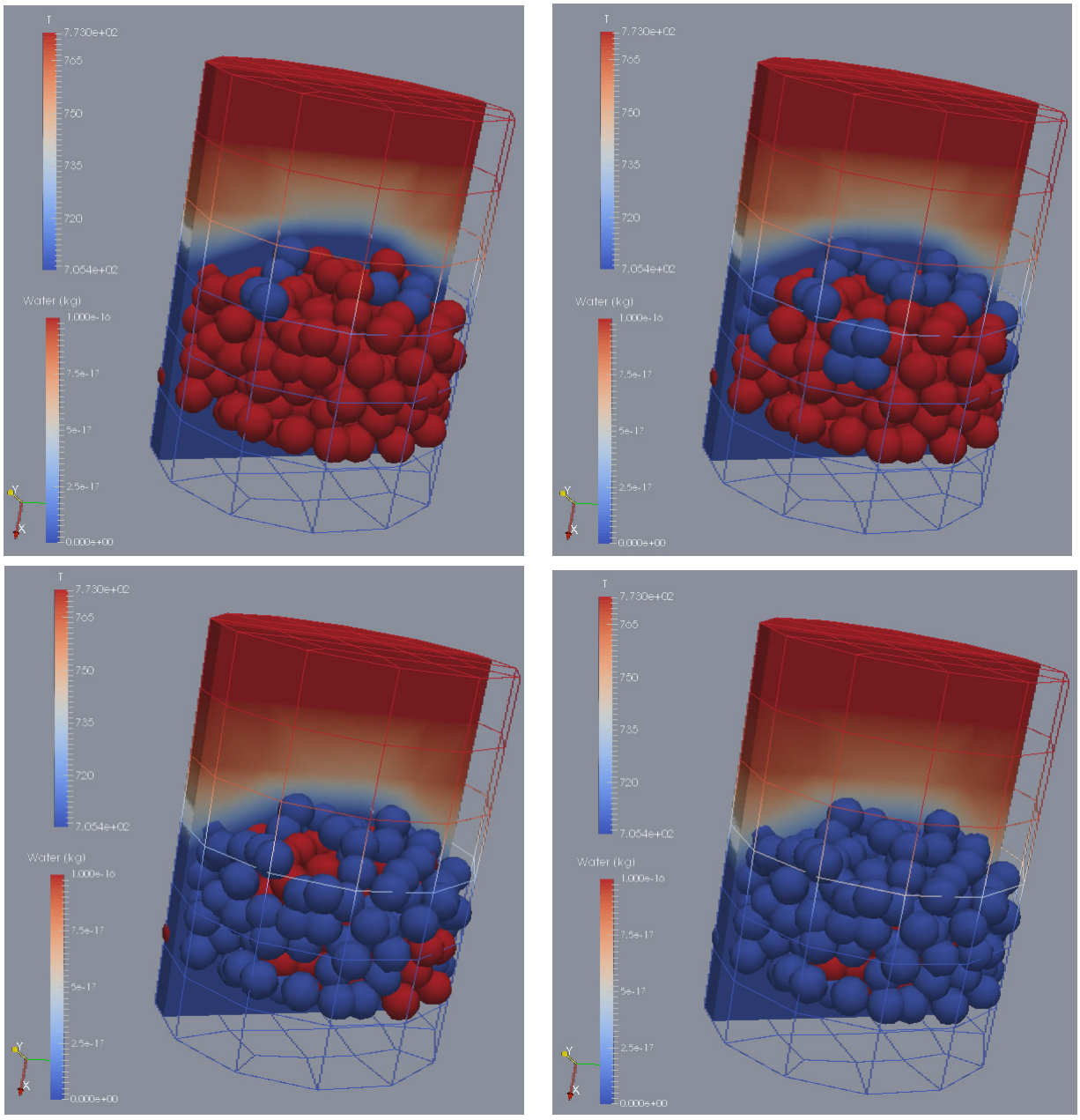

Figure 5: Water content in particles in different time steps in the simplified analysed reactor

6 NUMERICAL SIMULATIONS - ANSYS FLUENT

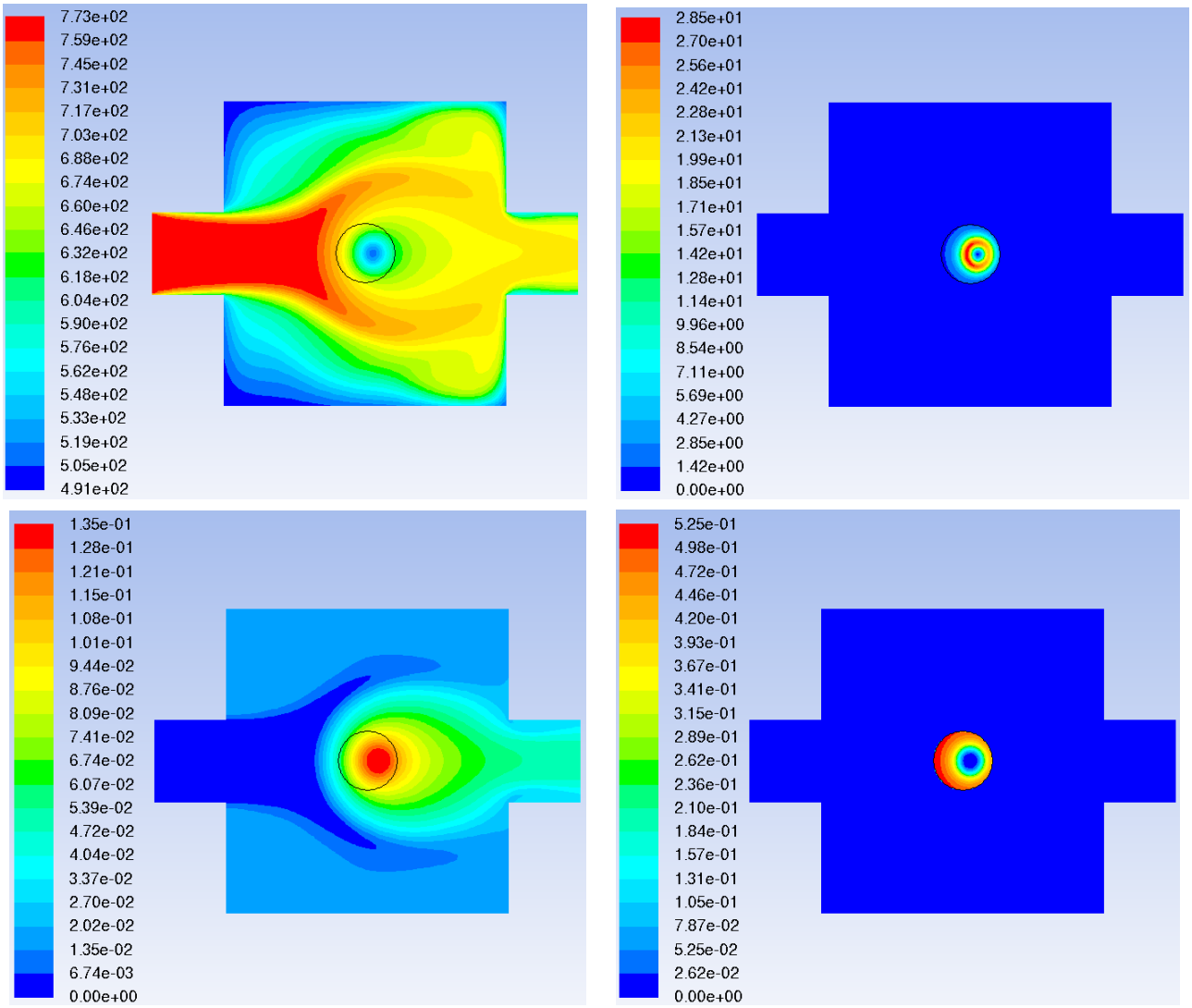

Figure 6: Particle parameters after 30 s of heating: temperature and gas mass source (top), volatiles mass fraction and porosity (bottom)

For comparison the numerical analysis of single wood particle heating obtained from ANSYS FLUENT is presented. The cold particle with diameter of 9 mm is heated by the stream of hot nitrogen. Temperatures of solid and gas are assumed to be at 298 K and 773 K, respectively. Gas inlet velocity was set to 2.3 m/s. Due to the heat transfer from the surrounding gases, the structure of particle is changing and the volatiles are released. The volatiles mass source term, the porosity and the wood density variation were implemented to the ANSYS FLUENT code by UDF function basing on the appropriate temperature

dependencies [9].

In Fig.6 the propagation of the heating front can be observed. The temperature of the particle is changing asymmetrically according to the hot gas flow direction. The average temperature of the particle at chosen time is ca. 620 K, which is the temperature the most intense pyrolysis for pine wood (data from TGA, [9]). Due to the increase of particle temperature the volatiles are released, what can be seen from the pictures showing the gas mass source (top right picture) and the mass fraction of released volatiles (bottom left picture). Gas mass source has a maximum value at the places corresponding to the particle temperature of 600 K. There is no gas release inside the particle, where its temperature is below 500 K. From the distribution of volatiles mass fraction, it can be observed that there is some kind of a gas-bag formed around the particle, which slows down the temperature propagation into the wood. Due to mass loss, also the porosity of wood is changing: from 0% in the colder parts to the 52.5% in the devolatilized parts of the analysed particle (right picture, at the bottom).

In the future this results can be compared with the single solid fuel particle analysis obtained from XDEM.

7 CONCLUSIONS

The main goal of this work was to investigate the possibility of the XDEM program to simulate the behaviour of wood particles during the gasification process that was performed in the real gasifier called INKA (IMP PAN). Basing on the test case calculations of the analysed gasifier, the following conclusions can be made:

- the XDEM method can be used to simulate heat and mass transfer processes in the biomass packed bed reactors, but it has some limitations concerning the number of the analysed particles,
- due to the computation time only the simplified geometries should be taken into account,
- the test case with the simplified geometry includes 300 particles, but the results with calculated temperature field and moisture content could be extended to large number of particles,
- the numerical results show propagation of the heating front and the change of the moisture content in each particle,
- to get better results at the first stage of the analysis using coupled XDEM/CFD, the behaviour of single particle during the gasification process should be considered,
- the single solid fuel particle XDEM analysis can be compared with other CFD simulations.

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